Reaction of a new metal organic complex by water's action on Cu(110)

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The control over the functionality, size and shape of new nanostructures is a mayor goal in nanoscience[1]. The bottom up strategies for forming on surface nanostructures by direct sublimation of their building blocks under UHV conditions has been shown as an excellent approach to this goal[2]. The stability for the molecule to allow sublimation without structural damage presents a limitation.

For this reason, in most of previous studies of large complex molecules on surfaces the molecules were transferred from a solution or by a dry imprint technique to the substrate in order to preserve the fragile core[3]. In this work we focus on a transition metal complex $[Cu_4(\mu_3\text{-}Cl)_4(\mu\text{-}pym_2S_2)_4]$ (pym_2S_2= dipyrimidinedisulfide) (named Cu4) with a robust structure [Fig.1a]. We have shown to be able to sublimate them keeping its molecular integrity and how they self-assemble without being disrupted by the surface[4] [Fig. 1b]. The transformation of these huge metal-organic molecules in solution[5] is clearly altered by the role of the substrate. We have observed *in situ* how the self-assembled molecular chains transform into other smaller chains by water's action [Fig. 1c].

The combination of surface techniques LEED, STM-VT, XPS and DFT calculations let us to the understanding of the reaction between Cu4 molecules and the Cu(110) substrate by water action. The new formed structure exhibits chains that are 60˚ rotated respect to the original ones. We propose a model for such a structure corresponding to a new polymeric bidimensional metal-organic compound of formula $[Cu(\mu\text{-}pym_2S_2)(\mu\text{-}Cl)]_n$.

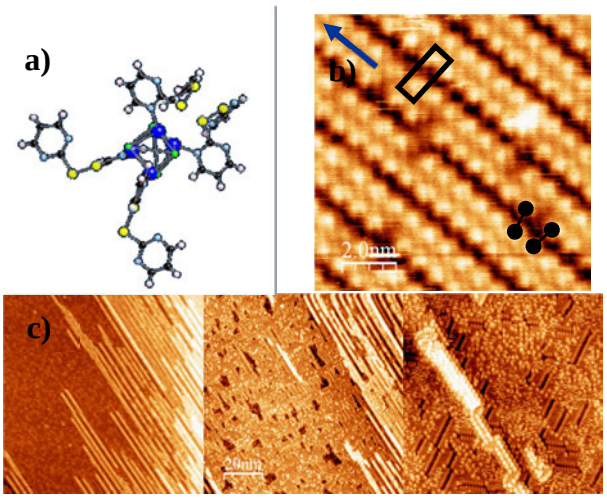

Figure: a) Representation of the $[Cu_4(\mu_3\text{-}Cl)_4(\mu\text{-}pym_2S_2)_4]$ molecule. b) STM image with molecular resolution where each two lobes correspond to one Cu4 molecule. c) STM images corresponding to different moments of the water adsorption on Cu4 covered Cu(110) surface. Left: Cu4 covered surface. Middle: during water adsorption of the same area. Right: after reaction of the water with the substrate and the metal-organic molecules.

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